MICROWAVE SPECTROSCOPY STUDY SUPPORTED BY QUANTUM CHEMISTRY CALCULATIONS OF LIMONA KETONE, A KEY OXIDATION PRODUCT OF LIMONENE

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Vegetation is a major source of emission of Biogenic Volatile Organic Compounds (BVOCs), which play an important role in atmospheric chemistry. Apart from methane and isoprene, monoterpenes ($C_{10}H_{16}$) are emitted in significant amounts by plants. Among these, α-pinene, β-pinene, and limonene are the predominant species[a]. Recently, limonene and limonene oxide have been studied extensively with Fourier transform microwave spectroscopy (FTMW)[b,c]. Limona ketone ($C_9H_{14}O$) is a major oxidation product of limonene, and it was shown that it is considered as precursor of Secondary Organic Aerosol (SOA) formation[d]. Thus, BVOCs have considerable impact on numerous environmental processes, climate, and health, and it is important to determine their gas phase structure and to predict their interaction sites and patterns with surrounding molecular systems. Within this context, the rotational spectrum of limona ketone was recorded and analyzed over the 3.8-19.3 GHz range using FTMW spectrometer[e]. The rotational spectrum analysis was supported by quantum chemical calculations, and transitions were assigned to the most stable equatorial conformer. The spectrum showed clearly that the lines were split. This splitting is due to internal rotation of methyl group, where the A and E states lines were assigned and fitted at instrumental accuracy, and the experimental barrier of the methyl torsion was determined.

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